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Two-Level System Coupled to Phonons: A Discrete Path-Integral Method

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A discrete path-integral representation for the partition function of a two-level tunneling system coupled to acoustic phonons is derived. This representation allows calculation of properties in the whole coupling range. As a function of the coupling there is an abrupt (ground-state) transition from the weak-coupling regime to the self-trapped state. From a moment analysis of the time-dependent spin-correlation function it follows that there is loss of phase coherence if the coupling exceeds the critical coupling. In this regime the mean effective tunneling rate vanishes linearly with temperature.

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We consider a two-level system represented by Pauli spin matrices which is coupled to a thermal bath of bosons, e.g., phonons.[1-5] For one-dimensional phonons the Hamiltonian reads

$$H=-h\sigma^x+\sum_k[\omega_k a_k^\dagger a_k+\sigma^z(B_k a_k^\dagger+B_k^* a_k)], \quad (1)$$

with $\sigma^\alpha\sigma^\beta=i\epsilon_{\alpha\beta\gamma}\sigma^\gamma$. Extending (1) to two- or three-dimensional phonons is straightforward. The Hamiltonian (1) bears strong resemblance to those discussed in connection with the polaron problem[6] and the Kondo effect, is important for the understanding of paraelastic and paraelectric defects in solids, and can also be used to study the temperature dependence of the tunnel splitting of rotators caused by rotator-phonon coupling.[7] Recently models very similar to (1) have been used to describe macroscopic tunneling in Josephson junctions and SQUID's.[8-13] The model (1) represents the simplest system where as a result of the coupling to a many-body system (and not because of a selection rule) transitions between two states of equal energy can take a very long time.

The system described by (1) exhibits two regimes with different physical behavior. In the strong-coupling limit, the spin is trapped in a field built by the phonons and it takes a long time before the spin flips from one state to another. In the small-coupling limit the spin tunnels with frequency $2h$. In the intermediate-coupling regime there is a transition from a nearly free to a self-trapped state.[3-5] Except for the case of a single-phonon mode for which H can be diagonalized exactly[4,14] all treatments are approximate.[1-5,8-10]

In order to calculate the properties of (1) for a wide range of temperatures and *all* values of the coupling we use the generalized Trotter formula[15] to write the partition function as a discrete path integral. We have

$$Z=\lim_{m\to\infty} Z_m, \quad (2a)$$

$$Z_m=\mathrm{Tr}[\exp(-\tau H_1)\exp(-\tau H_2)\exp(-\tau H_3)]^m, \quad (2b)$$

where H_1, H_2, and H_3 correspond to the three terms in (1) and $\tau=\beta/m$. We evaluate the approximation Z_m by inserting complete sets of states (labeled by Greek subscripts in the following) between the m factors. For the spin we use the eigenstates of σ^z. Because the spin-phonon coupling is bilinear in the phonon coordinates, the phonons can be integrated out.[16] If $S_\alpha=\pm 1$ denotes an Ising spin variable and $J=\frac{1}{2}\ln\coth\tau h$ we use

$$\langle S_{\alpha-1}|\exp(\tau h\sigma^x)|S_\alpha\rangle=(\tfrac{1}{2}\sinh 2\tau h)^{1/2}\exp(JS_{\alpha-1}S_\alpha), \quad (3)$$

and we find

$$Z_m=Z_m{}^P Z_m{}^S, \quad (4)$$

$$Z_m{}^P=\prod_{\alpha=1}^m\prod_{k\neq 0}\left[\tau^2\omega_k{}^2+2\left(1-\cos\frac{2\pi\alpha}{m}\right)\right]^{-1/2}, \quad (5)$$

$$Z_m{}^S=(\tfrac{1}{2}\sinh 2\tau h)^{m/2}\sum_{\{S\alpha\}}\exp\left[J\sum_{\alpha=1}^m S_{\alpha-1}S_\alpha+\frac{1}{2}\sum_{\alpha=1}^m\sum_{\gamma=1}^m F(\alpha-\gamma)S_\alpha S_\gamma\right], \quad (6)$$

$$F(\alpha)=\sum_k|B_k|^2 I_k(\alpha), \quad (7)$$

$$I_k(\alpha)=\frac{2\tau^3\omega_k}{m}\sum_{\gamma=1}^m\left[\tau^2\omega_k{}^2+2\left(1-\cos\frac{2\pi\gamma}{m}\right)\right]^{-1}\cos\frac{2\pi\alpha\gamma}{m}. \quad (8)$$

Obviously $\lim_{m\to\infty} Z_m^P$ is the exact partition function of the unperturbed phonon system and the convergence of Z_m^P as a function of m can be studied by means of a simple computer program. The discrete path-integral representation Z_m^S is formally equivalent to the partition function of a chain of m Ising spins S_α with periodic boundary conditions, the length of the chain being given by m. The Ising spins interact through a nearest-neighbor coupling J (related to the field h) and through an effective long-range interaction $F(\alpha-\gamma)$ originating from the phonons.

Remark that the formal analogy with an Ising chain is merely suggestive and does not imply that one should simply use the techniques developed for classical statistical problems. The fact that the interactions J and $F(\alpha-\gamma)$ depend explicitly on the chain length m makes the calculation of Z_m^S much more subtle. In general this means that one cannot restrict oneself to a certain class of configurations; one has to sum them all. For example, putting $F(\alpha-\gamma)=0$ and solving (6) by means of the transfer-matrix technique leads to the conclusion that in order to recover the exact free-spin result one needs *all* eigenvalues of the transfer matrix, not just the largest.

Starting from Eqs. (6)–(8), deriving approximations for the thermodynamic quantities in terms of the Ising spins is straightforward. For example, the approximate (spin) energy is $E_m^S = -(1/m)(\partial/\partial\tau)\ln Z_m^S$ and the approximate longitudinal susceptibility is $\chi_m^z = \tau\sum_{\gamma=1}^m \langle S_\alpha S_{\alpha+\gamma}\rangle$.

The present method has two main advantages. In the first place it allows us to treat the complete coupling range in a unified manner and therefore makes it possible to study the transition between the small- and the large-coupling regime. Second it is very well suited for numerical calculations. Indeed with straightforward programming Z_m^S can be evaluated exactly for m values reaching up to about $m=20$ (the number of states to be summed over equals 2^m). If higher m values are needed we have to use the Monte Carlo simulation technique.[17] The only approximation made so far is to keep m finite. Therefore we have to study the convergence of the results as a function of m and extrapolate to $m\to\infty$ if necessary. Plots of the data as a function of $1/m$ reveal that to a very good approximation the results depend linearly on $1/m$, making extrapolations trivial.

We now discuss some of our numerical results. When the tunnel splitting $2h$ is taken as a unit the results are a function of three parameters: the reduced temperature $T/2h$, the binding energy $C/2h=\sum_k |B_k|^2/2h\omega_k$, and the maximum phonon frequency $\omega_m/2h$. We considered acoustic phonons with dispersion $\omega_k=\omega_m|\sin(k/2)|$ and coupling $B_k = i(C\omega_m^2\sin^2 k/2\omega_k)^{1/2}$ in one dimension, and Debye phonons $\omega_k=ck$ and coupling $B_k=i(C\omega_k)^{1/2}$ in three dimensions. For the parameter range covered we observed no qualitative nor important quantitative differences between the one- and three-dimensional cases. In the one-dimensional case our choice for ω_k and B_k leads to the same effective interaction as that of Refs. 8–10 provided one makes the same approximations as in Ref. 8 and identifies C with η.

In Fig. 1 we show the inverse longitudinal susceptibility $(\chi^z)^{-1}$ and the transverse susceptibility χ^x for $\omega_m=0.4h$, as functions of $C/2h$. In order to get reliable results for $T/2h=0.05$ we have to take large m values because for $m=20$, $2h\tau=1$. Therefore at this low temperature we did a Monte Carlo simulation for $m=100$. Our results clearly show that the transition from the low-coupling regime to the self-trapped state occurs around $C/2h=0.4$ and that the transition becomes sharper at lower temperature, suggesting a discontinuous transition in the ground state of the system.[3-5,9,10] In Fig. 2 we plot $\partial^2F^S/\partial C^2$ (where F^S denotes the spin free energy). This quantity measures the fluctuation of the spin-phonon coupling energy and consequently it should be very sensitive to changes of the coupling. The results for $\partial^2F^S/\partial C^2$ are in concert with those of Fig. 1 and lead

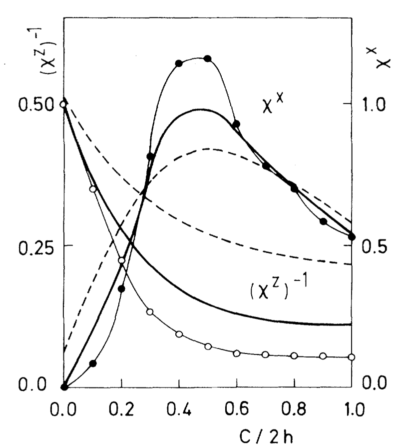

FIG. 1. Inverse longitudinal susceptibility $(\chi^z)^{-1}$ and transverse susceptibility χ^x as functions of the coupling $C/2h$ for $T/2h=0.2$ (dashed line) and $T/2h=0.1$ (solid line). The open circles and solid dots are Monte Carlo results corresponding to $(\chi^z)^{-1}$ and χ^x for $T/2h=0.05$ and $m=100$.

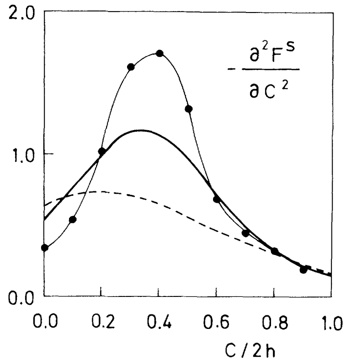

FIG. 2. The spin-phonon coupling-energy susceptibility for the same parameters as in Fig. 1.

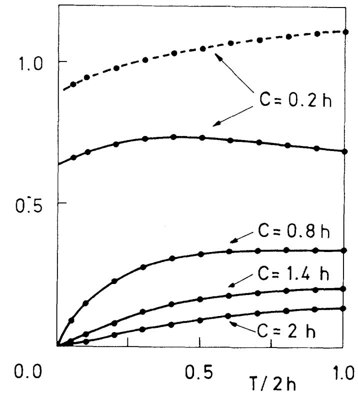

FIG. 3. The mean effective tunneling rate (solid line) given by Eq. (9) as a function of the temperature for several values of the coupling. The dashed line gives the tunnel frequency of the spin in the case of weak coupling. The solid line for the case $C/2h = 0.1$ is only shown to demonstrate that the temperature dependence of $\Delta_{\rm eff}$ (which is *not* the width of the resonances at the frequency given by the dashed line) in the weak-coupling regime is qualitatively different from that in the strong-coupling regime.

to the same conclusions concerning the nature of the transition. In the weak-coupling regime our results are in good agreement with mode-coupling theory.[5]

The effect of dissipation on the spin dynamics can be studied by calculating the longitudinal relaxation function $\Phi^z(t)$. As σ^z commutes with the spin-lattice interaction the problem is very similar to the problem of motional narrowing in magnetic resonance.[18] For weak coupling the spectrum of $\Phi^z(t)$ consists of two slightly broadened resonances centered around $\pm 2h$ (there is also a slight shift) and in addition there is a central resonance with a relatively small weight.[5] An estimate of the resonance frequency can be obtained from a moment analysis of the spectral function and a typical weak-coupling result is given in Fig. 3 (dashed line). In the strong-coupling regime the clocklike motion of σ^z turns into a stochastic tunneling process and the spectral response function is dominated by a Lorentzian centered around frequency zero. The width of this central resonance (the mean effective tunneling rate) is then proportional to[18]

$$\Delta_{\rm eff} = 2h^{1/2}(\chi^z)^{-1}\langle\sigma^x\rangle^{3/2}(h\langle\sigma^x\rangle - 2C\partial F^S/\partial C)^{-1/2}. \tag{9}$$

In Fig. 3 we have plotted $\Delta_{\rm eff}$ as a function of the temperature for several values of the coupling. For strong coupling and low temperature a least-squares fit to *all* our data yields $\Delta_{\rm eff} \sim C^{-2}T$. In this regime the temperature dependence of $\Delta_{\rm eff}$ is determined by χ^z and a vanishing $\Delta_{\rm eff}$ is equivalent to a divergent χ^z (as $T \to 0$). We can compare this result with the prediction made by Bray and Moore. As mentioned before, their model is equivalent to ours in the one-dimensional case because the thermodynamics of the system are insensitive to the details of the phonon spectrum and the form of the coupling, as long as in the long-wavelength limit $k \to 0$ one has $\omega_k \sim k$ and $B_k \sim k^{1/2}$. Bray and Moore predict $\Delta_{\rm eff} \sim C^{-1}T^{aC-1}$ (a is an unimportant numerical factor), and they also find a vanishing $\Delta_{\rm eff}$ for strong coupling, but their result clearly differs from ours.

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